THERMAL SCIENCES

8 MAR 2012

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AFOSR / RSA
Air Force Research Laboratory

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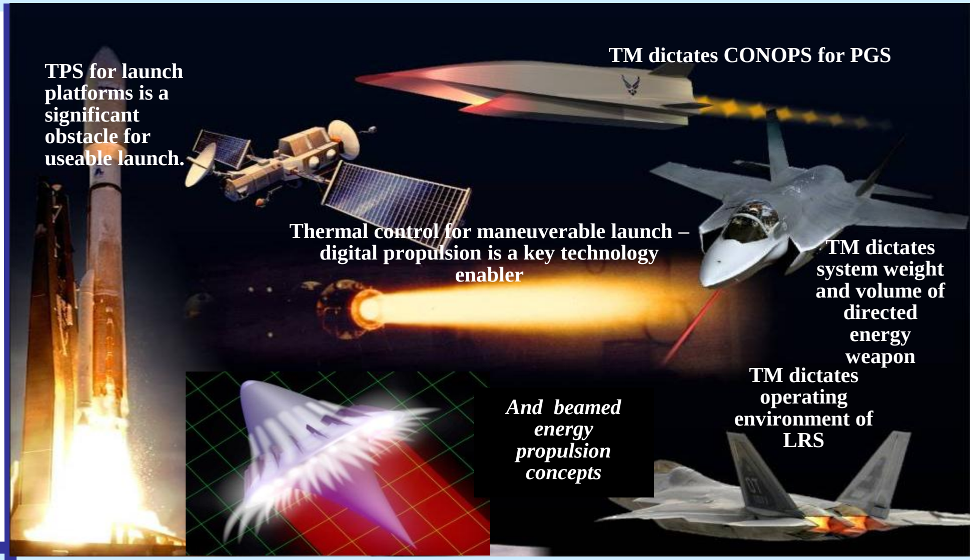
Energy, Power and Propulsion - 61102F
Thermal Sciences

MOTIVATION – Exploiting Phonons

- **The study of phonons - from nanoscale, microscale or larger scales – to enable the manipulation of phonons (aka *phononics) to enable a new technological frontier with a potential impact that could match that of electronics almost half a century ago.***

Thermal is the limiting factor for AF operations



SCIENTIFIC CHALLENGES

- **Developing the science base to understand and control of thermal transport in heterogeneous materials.**
- **Exploiting the interactions among phonons, photons and electrons and their interactions with surrounding material.**

PAYOFF

- **Ultra-low conductivity: dense materials with conductivity significantly below the predicted minimum for an isotropic solid.**
- **Techniques for controlling conductive thermal transport through excitation and manipulation of coherent phonons in a target materials.**

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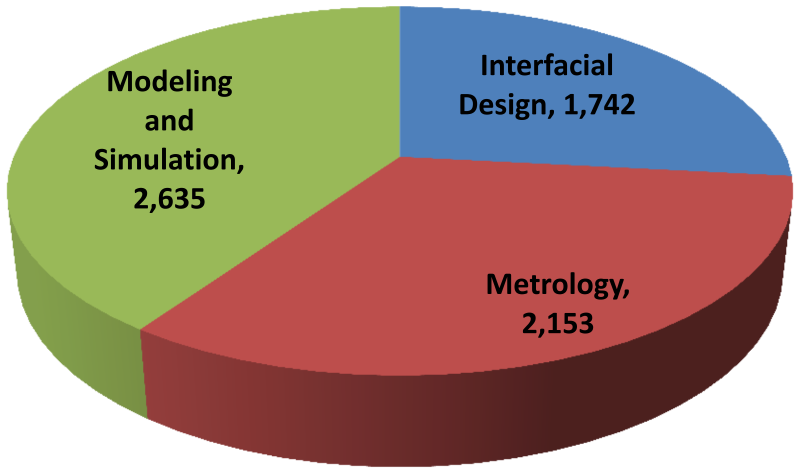
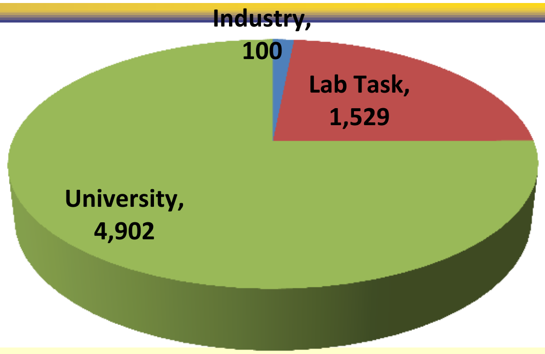




PE Code	FY11	FY12
61102F	4,052	4,206
61103F	2,379	2,449
65502F	100	100
	6,531	**6,754**

Distinguished Researchers:

- 7 Professional Society Fellows
- 1 Elsevier-Materials Science and Engineering Young Researcher Award
- 2011 Fritz London Memorial Prize Recipient
- ASME Orr Award, ASME Bergles-Rohsenow Award
- 8 NSF Career awardees
- 1NDSEG Fellowship
- 4 YIP winners
- 117 peer reviewed papers (over 3 year span).

Collaborations/Partnerships:

- **AFOSR Lead, AFRL Thermal Management Steering Committee**
- **Member of the ASD R&E Power and Energy COI**
- **Ongoing collaboration with NSF, ONR and DOE relevant programs**

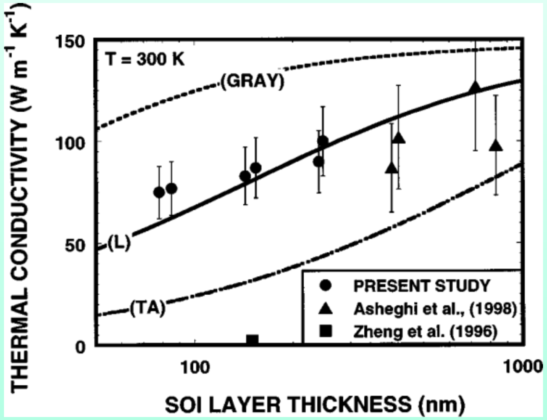
SCIENTIFIC CHALLENGES

- A leading fundamental problem is multicarrier interfacial transport (electron & phonon nonequilibrium), which is distinct from the single-carrier focus of most prior research.
- Another challenge is when one of the bounding media has nanoscale lateral dimensions, e.g., a nanowire or CNT contact.
- Both of these fundamental problems are complicated by materials (e.g., GeSbTe compounds for phase change memory) where both electrons and phonons contribute at comparable levels to the thermal conductivity.

Sub-area 1: Nano scale thermal transport – far field and near field

Scientific Gaps

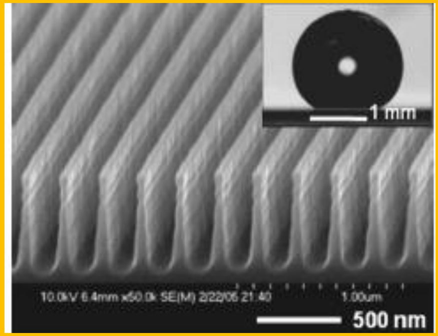
- Interface effects are not accounted for
  - Strain, lattice mismatch, atom mixing are neglected
- Discrepancy between predictions and experimental data remain
  - Phonon modes and polarization vectors are not considered
  - Contribution of long wavelength and small wavelength phonon modes are not decoupled
- Near field thermal transport phenomenon in general is poorly understood

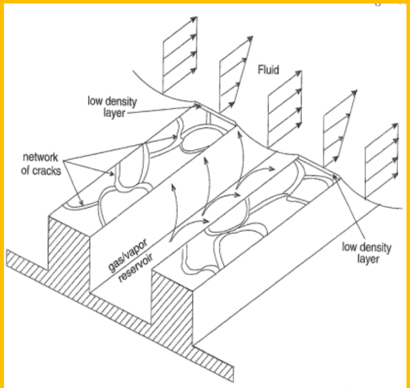


Discrepancy between experiment and prediction
Ju and Goodson, 1999

Sub area 2: Heat removal for large scale heat flux situations

- **Scientific Gaps:**
  - Current heat sinks are not capable of carrying away heat densities >100 W/cm^2
  - Physical mechanisms of convective heat transfer are unclear when surfaces are modified by nano structured features
  - Plenty of room for novel phase transformation concepts, but not being explored



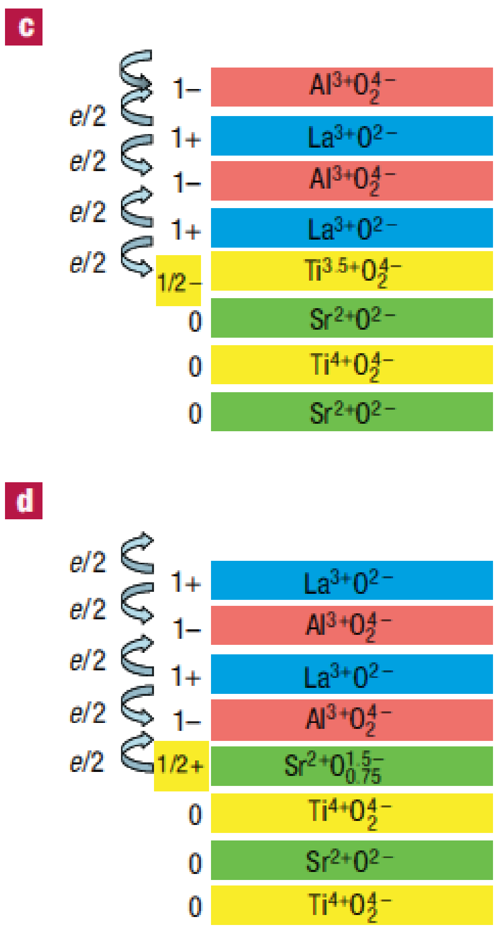


PI: Andy Williams
Space Vehicles Directorate

Sub Area 3: Thermal storage and conversion

Scientific Gaps

- How do we tackle irregular and massive thermal transients
  - Science-base to develop materials for high rates of thermal energy storage and release for thermal transients is lacking
  - Current thermal storage research is based on very traditional materials not suitable for future Air Force systems



Program Trends

Far field and near field thermal transport ↗

Heat removal for large scale heat flux situations ↘

Thermal storage and conversion ↘

REBRANDING the portfolio – Condensed Matter Physics with an emphasis on PHONONS

Other Organizations that Fund Related Work

- **DOE**
  - A major thrust is nanoscale science, where links between the electronic, optical, mechanical, and magnetic properties of nanostructures including strongly correlated electron systems, quantum transport, superconductivity, magnetism, and optics.
- **NSF**
  - Heat and mass transfer, biological and environment systems, large investment in thermoelectric materials for automobiles, broad engineering and societal impact
- **DARPA**
  - Thermal management technologies
- **ONR**
  - Nano lubricants, jet impingement, coolants, magnetic refrigeration, cooling power electronic modules, ship level thermal management tool
- **ARO**
  - Thermal management materials and novel thermal property characterization
- **ARPA-E**
  - Industrial and consumer related large scale storage issues

Current State of the art in understanding thermal transport

- Current SOA for thermal transport across and interface are based on the assumption that phonon transport proceeds via a combination of either ballistic or diffusive transport on either side of the interface.
  - Acoustic mismatch theory (AMM) (Little, 1959)
  - Diffuse mismatch theory (DMM) (Swartz and Pohl 1989)
- Both of these theories offer limited accuracy for nanoscale interfacial resistance predictions because of they neglect the atomic details of actual interfaces.
  - e.g. The AMM model assumes that phonons are transported across the interface w/o being scattered (ballistic)
  - And the DMM model assumes the opposite – that phonons are scattered diffusively.
- So in fact, these two models serve as upper and lower limits on the effect of scattering on the interfacial thermal resistance.

REALITY

- **BUT in both numerical and experimental studies in nanostructures ranging from *nanowires to polyethylene nanofibers* all show that phonons undergo <u>anomalous</u> diffusion**
- **- i.e. so termed superdiffusion -, being faster than normal diffusion but slower than ballistic transport.**
- **Therefore, it is necessary to establish an improved theory describing thermal transport across the interface by taking into account the anomalous thermal transport characteristics of nanostructures.**

Thermal Conductivity from First Principles

Alan McGaughey, YIP, CMU

Quantum-Mechanics Driven Prediction of Nanostructure Thermal Conductivity

- Quantum effects are important
  - Atomic interactions
  - Occupation numbers
- Bottom-up thermal conductivity prediction
  - Which modes dominate transport?
  - How to control scattering?
- Thermal transport in nanostructures
  - Strategies for tailoring properties
  - Multi-physics challenges

- **Describing the atomic interactions**

Taylor expansion about the equilibrium energy E_0 and N atoms

Goes to zero

$$E = E_0 + \cancel{\sum_i \sum_\alpha \left.\frac{\partial E}{\partial u_{i,\alpha}}\right|_0 u_{i,\alpha}} + \frac{1}{2} \sum_{i,j} \sum_{\alpha,\beta} \left.\frac{\partial^2 E}{\partial u_{i,\alpha} \partial u_{j,\beta}}\right|_0 u_{i,\alpha} u_{j,\beta} + \frac{1}{6} \sum_{i,j,k} \sum_{\alpha,\beta,\gamma} \left.\frac{\partial^3 E}{\partial u_{i,\alpha} \partial u_{j,\beta} \partial u_{k,\gamma}}\right|_0 u_{i,\alpha} u_{j,\beta} u_{k,\gamma} + \ldots$$

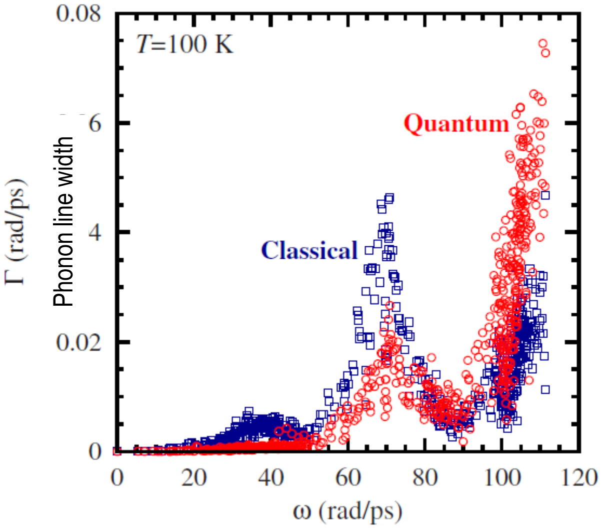
Harmonic force constant

Anharmonic term: Phonon properties are obtained from here

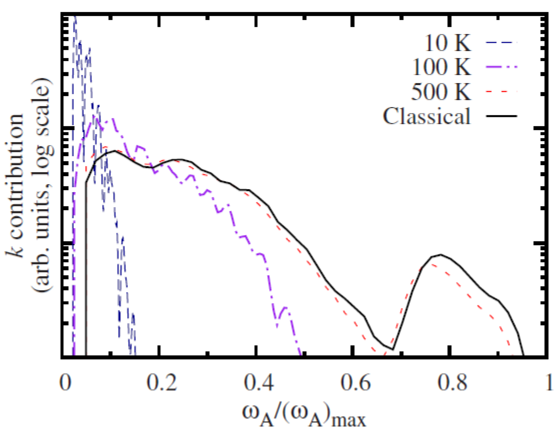
- Force constants can come from empirical potentials or quantum mechanics
- Used in anharmonic lattice dynamics calculations to predict phonon properties

Thermal Conductivity from First Principles

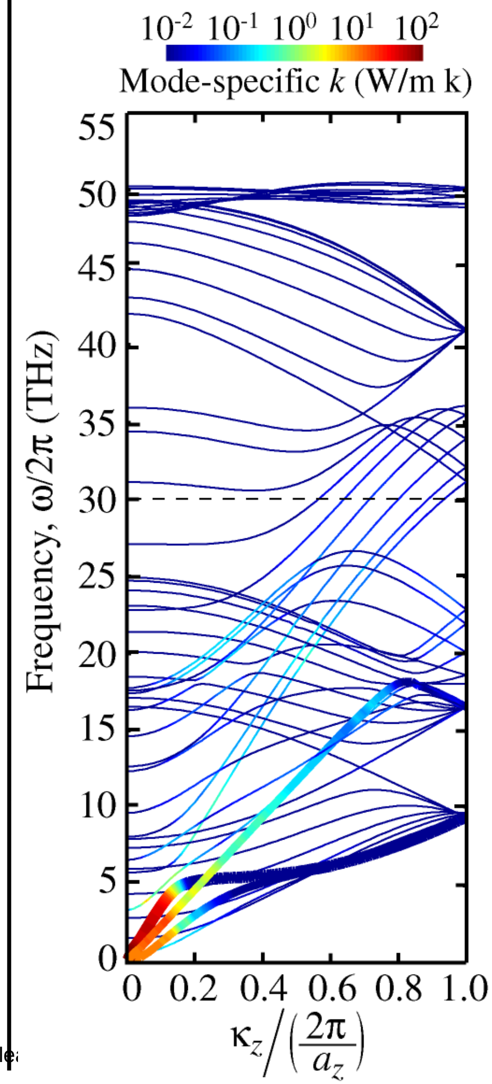
- Phonon occupation number
  - specific heat and scattering



Contribution to thermal conductivity (Si)



- Phonon properties from the spectral energy density (CNT)

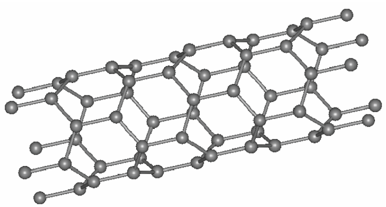


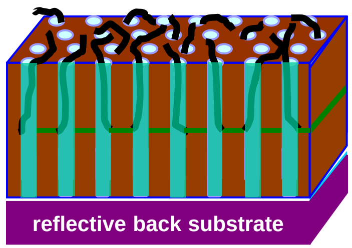
	Empty	Water filled
Acoustic	173	97
Optical (low)	196	190
Optical (high)	24	24
Total SED	393	311
Total NEMD	407	300

Thermal Transport Transfer

Ruan and Fisher-- Purdue

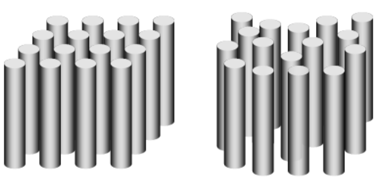
***ab initio* and experiments to understand near field thermal transport in CNT arrays**



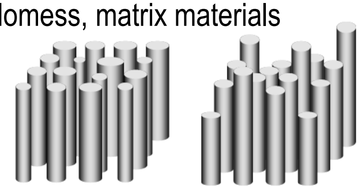


atomic scale effects: chirality, doping

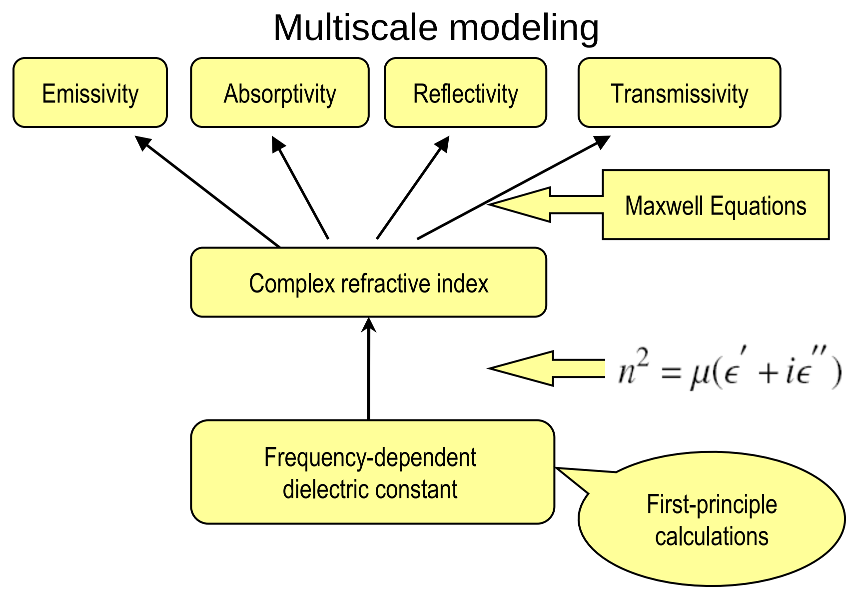
nano scale effects: periodicity, randomess, matrix materials



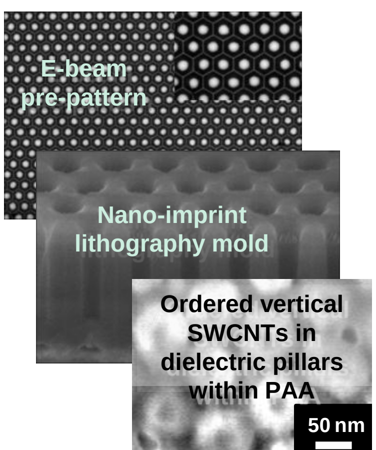
Ordered   Random Position

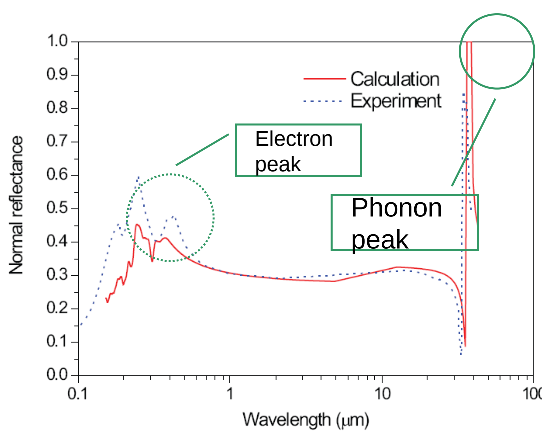


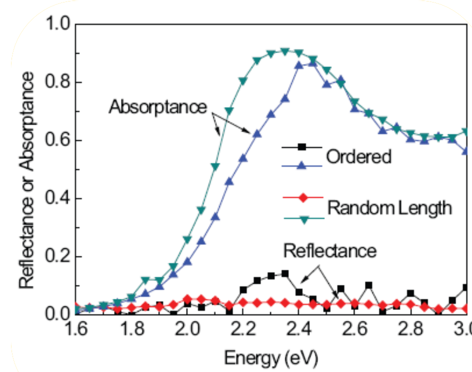
Random Diameter   Random Length



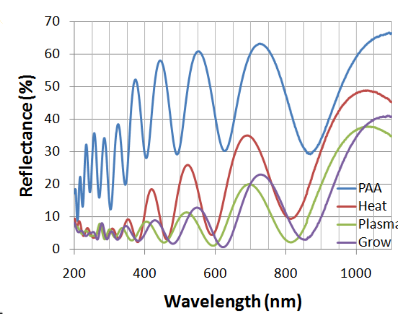
Synthesis of patterned vertical CNT arrays







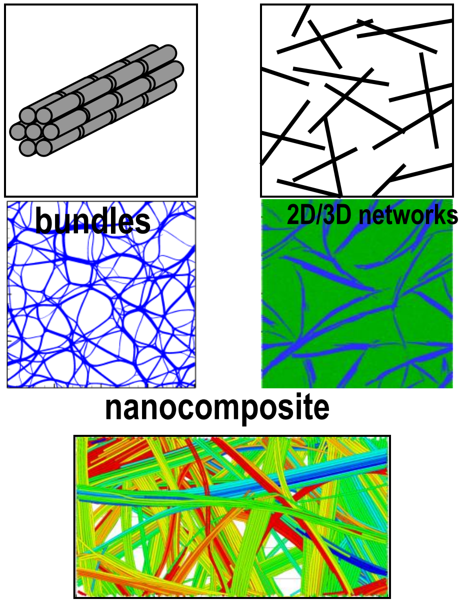
(a) $f = 0.2$



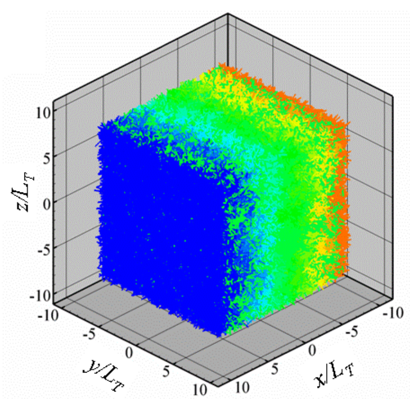
Nano scale Enabled Thermal Transport

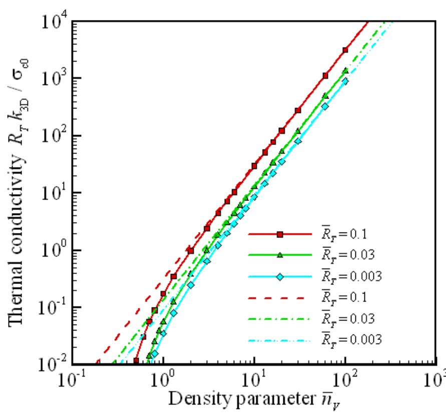
Leonid Zhigilei, UVA

Mesoscopic Modeling of Heat Transfer in Nanofibrous Materials



- Develop a mesoscopic model capable of modeling structural self-organization and thermal transport in nanofibrous materials
- Account for
  - Interfacial CNT-CNT and CNT-matrix heat transfer → parameterization of the mesoscopic model
  - Nanofibrous structures of increasing complexity
  - Monte Carlo calculation of statistical averages for quantities entering the theoretical equations



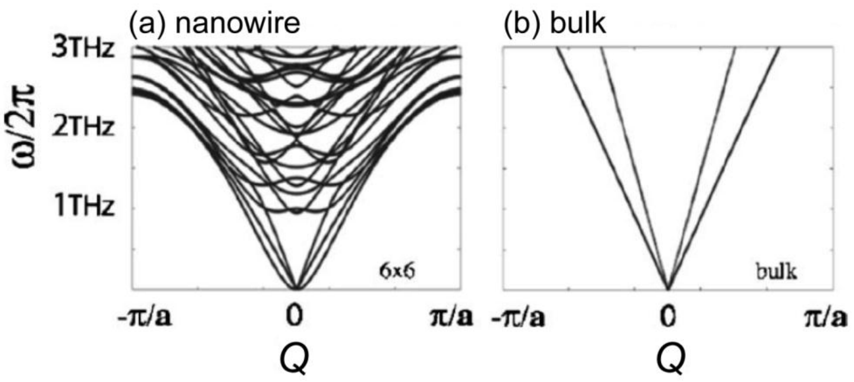


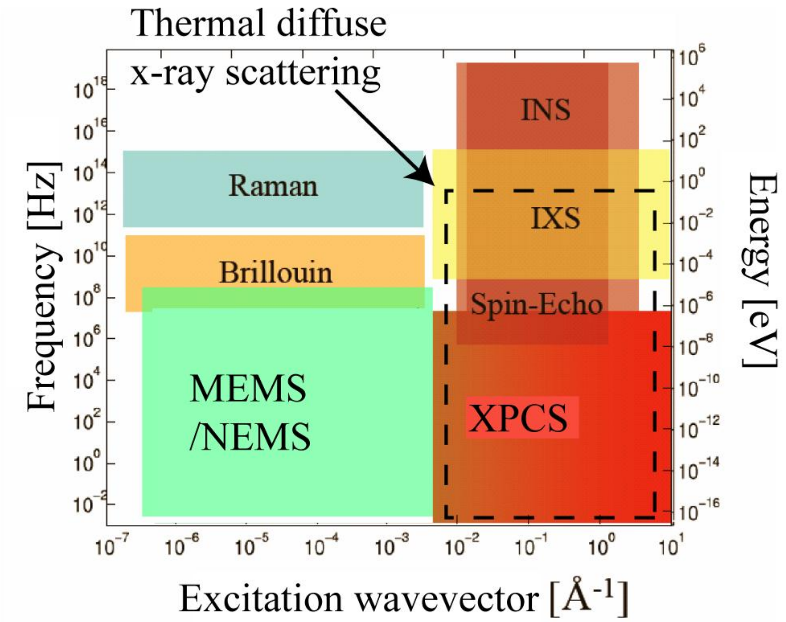
- Atomistic MD simulations of energy dissipation and heat transfer in individual CNTs are performed and are being extended to groups of interacting CNTs
- Scaling laws for thermal conductivity of straight bundles and isotropic networks of straight nanofibers are derived analytically and verified in Monte Carlo simulations

Phonon Modes Characterization

Paul Evans-- University of Wisconsin Martin Holt-- Argonne

New low-frequency zone boundary modes



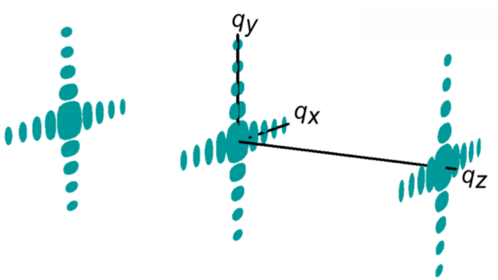


Phonon characterization

- **Zone boundary phonons require large momentum transfer**
- **Visible photons don't have enough momentum**
- **Inelastic x-ray and neutron scattering require large volumes**
- **Thermal diffuse x-ray scattering offers the potential to probe modest volumes with large momentum transfers**

Phonon modes relevant to thermal properties can have large Q

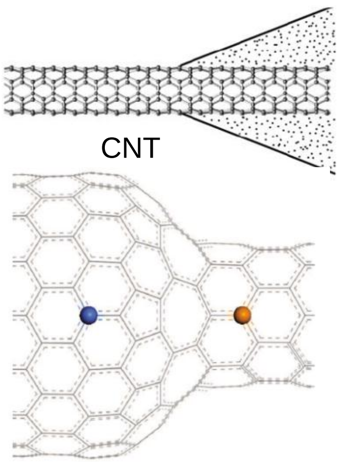
- **Nanowire q_z spans entire Brillouin zone, up to 1 Å^{-1}**

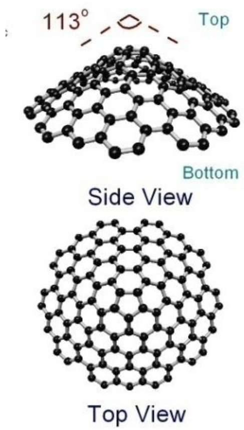


Near Field Thermal Transport

Cahill, UIUC, MURI

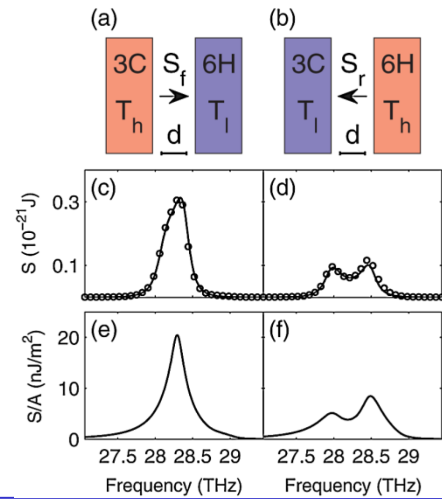
Prior work (2006, 2007)





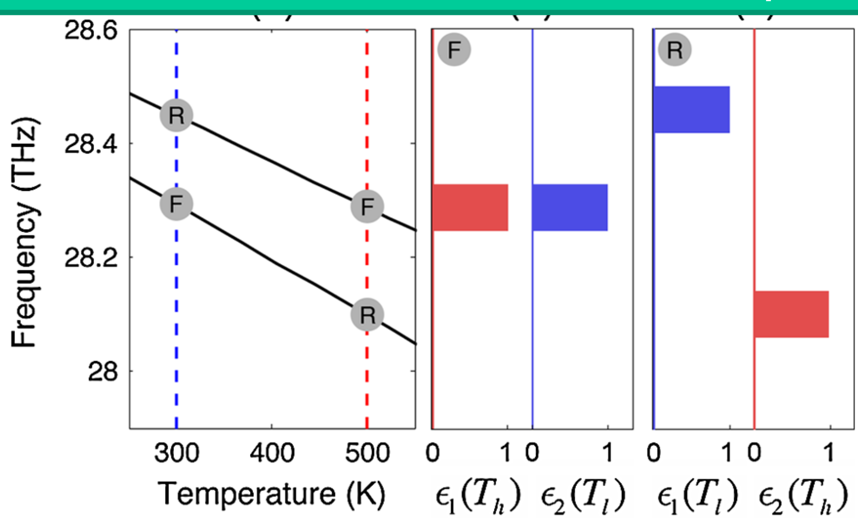
Nano cone

Otey, et al., in print, PRL, 2011



Physical mechanism for thermal diode is understood by the match /mismatch phonon's DOS spectra

Thermal rectification in near field radiation transport



Potential Phononic Devices

- Phonon is used to carry and process information
- Thermal rectification plays the most central role in phononics devices

AFRL

Homeland Security NewsWire

- **Shape of things to come-- Phononic computer processes information with heat**

- **In addition to electronic computers and (theoretical) optical computers, we now have heat-based computers; such computers are based on logic gates in which inputs and outputs are represented by different temperatures; in run-of-the-mill electronic computers, inputs and outputs are represented by different voltages.**

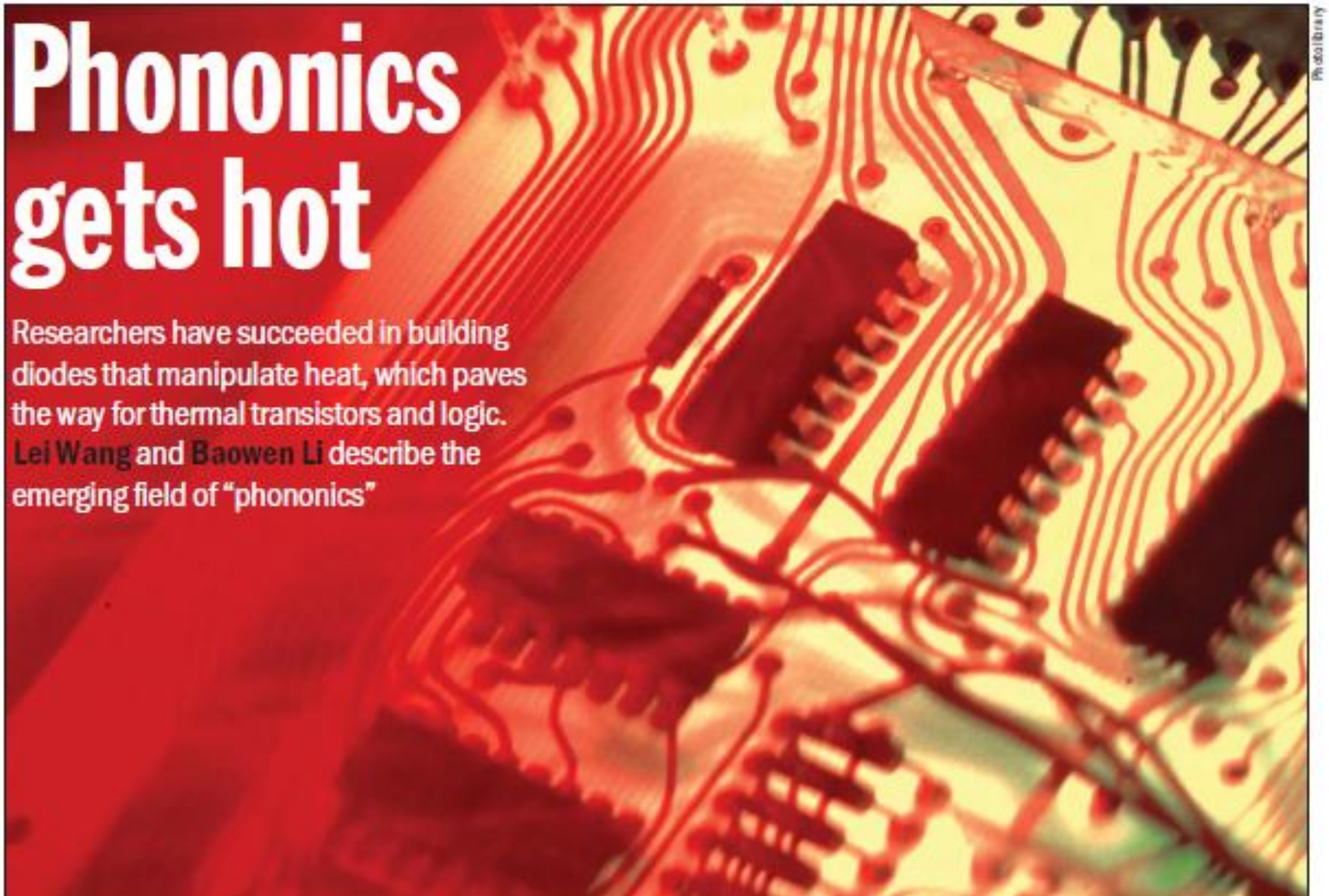
Prototype thermal transistors and thermal logic gates – perhaps even thermal computers – will be available in the near future

Physics World, 2008

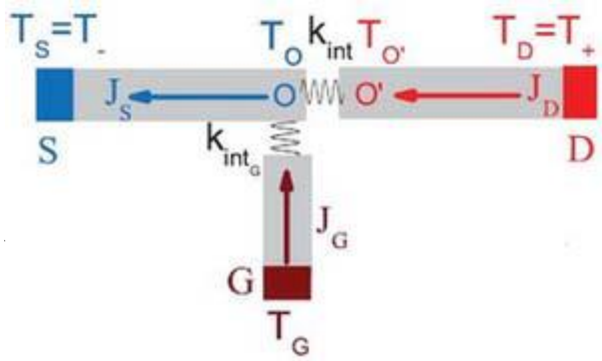
Dr. Baowen Li, University of Singapore – world leader

physicsworld.com

Feature: Thermal logic



Phononics: Manipulating heat flow with electronic analogues and beyond



- **Heat due to lattice vibration is usually regarded as harmful for information processing. However, studies in recent have challenged this mindset.**
- **Baowen Li (University of Singapore) has recently reported/demonstrated via numerical simulation, theoretical analysis and experiments that phonons can be manipulated like electrons. They can be used to carry and process information.**

Colloquium: Phononics Coming to Life: Manipulating Nanoscale Heat Transport and Beyond , *Physical Review Letters*, 2011

Thermal Sciences 2012

- **Exciting, rapidly expanding multidisciplinary community.**
- **Supporting the world's leading theorists and experimentalist.**
- **Exploring new phononic phenomena and …**
- **Creating new experimental tools**
- **With the goal of enhancing the AF of tomorrow!**